CHEMICAL RESEARCH, DEVELOPMENT & ENGINEERING CENTER

CRDEC-SP-88032

DATA BASE USERS' GUIDE FOR THE CHEMICAL AGENT SIMULANT DATA CENTER

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U.S. ARMY ARMAMENT MUNITIONS CHEMICAL COMMAND

Aberdeen Proving Ground, Maryland 21010-5423

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Computerized data base of important property data associated with compounds used as chemical agent simulants.

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The Chemical Agent Simulant Data Center (CASDC) established a computerized data base on compounds that were used, recommended, screened, or otherwise considered as chemical agent simulants. It is an on-line, user-friendly data base that is available to CRDEC personnel, DOD services, other government agencies, and their contractors. Currently there are over 600 simulant related compounds having 50 different types of data that can be searched. The report describes accessibility and datatypes, explains how to conduct searches and generate reports, and lists who to contact for assistance.

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PREFACE

The work described in this report was authorized under Project No. 1L162706A553, Chemical Detection and Identification Technology. This work was started in September 1982 and is continuing.

The use of trade names or manufacturers' names in this report does not constitute an official endorsement of any commercial products. This report may not be cited for purposes of advertisement.

This report has been approved for release to the public.

Acknowledgments

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DATA BASE USERS' GUIDE FOR THE CHEMICAL AGENT SIMULANT DATA CENTER

1. INTRODUCTION

The increasing difficulties associated with open air testing with toxic chemicals requires the use of less toxic simulants to minimize adverse environmental impacts. Simulants can also reduce the hazard to laboratory personnel and the cost of waste disposal. Because any compound that is not a surety compound is a potential simulant, the selection process for an optimum simulant can be overwhelming. Fortunately, computers and computer data bases are available or can be established to simplify the search.

The U.S. Army Chemical Research, Development and Engineering Center (CRDEC), other Department of Defense organizations, and contractors engaged in simulant research recognized the need for a centralized data repository. The requirements are (1) quick access to pertinent data, (2) literature references, (3) identification of data gaps, (4) and the capability to identify and resolve conflicting data. CRDEC, as the lead organization in simulation of toxic chemical warfare (CW) agents, established the Chemical Agent Simulant Data Center (CASDC) in response to that need.

A simulant cannot exactly match all the physical/chemical properties of a chemical agent. The structural features that determine toxicity usually have the greatest influence on physical/chemical property determination. The data base, therefore, has numerous organophosphorus compounds for screening nerve agent simulants, sulfides for mustard simulants, or other compounds of the same chemical class as the compound to be simulated. The CASDC allows you to search for structural features and physical/chemical properties, thereby permitting structure versus property correlation analysis. The data base should contain as many potential simulant compounds as possible to increase the probability of identifying the chemical that most closely matches the properties of the agent. The listing should have a preponderance of chemicals that have available property data, have been screened for toxicity, and have environmental impact data available to diminish the cost of providing the required information.

The purpose of the CASDC is to assist simulant users in choosing and employing simulants through the compilation of a comprehensive data base on related compounds. It must also provide a quick and practical method to access the data. The CASDC makes a simulant recommendation for a particular application

after a rational evaluation of essential properties; however, it does not certify or approve simulants for release into the environment. It also does not serve as a clearing center for simulant use permission. The final decision regarding simulant use is the responsibility of the principal scientist overseeing the investigation.

2. METHODS

2.1 Literature Sources

Through examination of CRDEC bibliographies in CRDEC's Technical Library, automated literature searches through the Defense Technical Information Center's data base, and cited references in simulant related literature, a bibliography of 1,000 references was compiled. Sources include DOD services and other government agencies, private contractors, foreign sources, and the open literature. Various research and testing activities use simulants for spray, explosive and bulk dissemination; standard and experimental methods of decontamination; different methods of agent detection and identification; troop training and trialing to include a total intake simulant; collective protection studies; pick-up and transfer studies; and contamination avoidance. These are general simulant application descriptions and may require different simulants for specific applications within each activity.

The initial search strategy was to address a single application at a time beginning with dissemination. These simulants were the first used and recently have been recommended for other applications. As a result of numerous queries to the CASDC, it became clear that all applications should be examined, with emphasis on recency, so that state-of-the-art in simulant research could be reflected. This required the determination of what agents, applications, and properties have been considered in simulant research.

Simulant compilations were examined first so that a listing could be generated quickly. After initial identification and data extraction, various standard chemical data sources were examined to amass as much data as possible. Numerous compounds were added to the data base by recommendations from simulant researchers with further data gleaned from standard chemical references.

2.2 Datatypes

To identify the types of data to be incorporated into the data base, a preliminary review of simulant literature and interviews with key simulant researchers was done. As a result we decided to include as many physical/chemical properties as possible to accommodate various simulant applications and to ensure that unforeseen future property data needs are met. The data base also required the

inclusion of data at different conditions for dependent variables and conflicting data from different sources. Various simulant applications require the matching of one or more properties judged essential for duplicating the agent in an experiment. The properties list is, therefore, a summation of essential properties covering all simulant applications. Table 1 lists the datatypes number, field name, field type, and units label in the order in which they appear in the data base. New datatypes will be added as they are identified. An effort is made to standardize units of measure and to state dependent variables wherever possible. Originators of other data bases within CRDEC should attempt to use common units of measure that will simplify queries and data transfer among various data bases.

2.3 Property Estimations

To fill some of the data gaps in the data base, property estimation routines are employed. These estimates are used until other sources for the data have been encountered. The routines are derived from open literature, computer programs, or developed by personnel in the Chemometrics and Biometrics Modeling Branch (CBM), Physics Division, Research Directorate, CRDEC. Estimated data is appropriately noted with an insertion of "est" in the comments field. This type of data can also be discerned because all data estimations or calculations generated by CBM personnel use reference citation 54. Diminishing the number of data gaps helps increase the probability that the most appropriate candidate simulant will be identified. The CASDC uses estimation routines for the following properties:

vapor pressure	volatility
surface tension	density
vapor density	boiling point
heat of vaporization	heat of formation
heat capacity	viscosity
water solubility	octanol/water partition coefficient
refractive index	Hildebrandt solubility parameter
molar volume	molar refraction

2.4 Data Base Management System

The CASDC was initially located on the CRDEC's Univac 1108 computer using CREAT-A-BASE (Level 5E) management software (NDX Corporation,

TABLE 1. INDEX OF DATATYPES

Datatype Number	Field Name	Field Type	Units Label
Fixed Datatypes			
1	CRDEC Number	CRDEC-00000	
2	Date Entered	MM/DD/YY	
3	Molecular Weight	Numeric	
4	CAS Registry Number	00000-00-0	
5	Wiswesser Line-Notation	Text	
6	Military Designation	Text	
Flexible Datatypes			
7	Synonyms	Text	
8	Vapor Pressure	Numeric	Torr
9	Density	Numeric	g/cm^3
10	Vapor Density	Numeric	Air=1
11	Boiling Point	Numeric	°C
12	Melting Point	Numeric	°C
13	Molar Volume	Numeric	$cm^3/mole$
14	Surface Tension	Numeric	dynes/cm
15	Viscosity	Numeric	centipoise
16	Vapor Viscosity	Numeric	micropoise
17	Volatility	Numeric	mg/m^3
18	Diffusion Coefficient	Numeric	cm^2/s
19	Refractive Index	Numeric	sodium D line
20	Molar Refraction	Numeric	cm^3/gm mole
21	Decomposition Temperature	Numeric	°C
22	Flash Point	Numeric	°C
23	Autoignition Temperature	Numeric	°C

24	Oxygen Index	Numeric	%
25	Heat of Vaporization	Numeric	cal/gm
26	Heat of Combustion	Numeric	cal/gm
27	Heat of Fusion	Numeric	cal/gm
28	Heat of Formation	Numeric	cal/gm
29	Energy of Vaporization	Numeric	cal/gm
30	Heat Capacity	Numeric	cal/gm °C
31	Specific Heat	Numeric	cal/gm °C
32	Hydrolysis Rate	Text	
33	Oct/Water Partition Coefficient	Numeric	Log P
34	Hildebrandt Solubility Parameter	Numeric	$(cal/cm^3)^{1/2}$
35	Hygroscopicity	Text	
36	Water Solubility	Text	
37	Water Solubility Value	Numeric	gm/100 mL
38	Critical Temperature	Numeric	°C
39	Critical Pressure	Numeric	Atmospheres
40	Critical Volume	Numeric	$cm^3/mole$
41	Critical Density	Numeric	gm/cm^3
42	Dielectric Constant	Numeric	Dimensionless
43	Dipole Moment	Numeric	debyes
44	Toxicity	Text	
45	Chemical Reactivity	Text	
46	Simulant Application	Text	
47	Industrial Application	Text	
48	Comments	Text	

Houston, TX). The decision to make the CASDC an on-line accessible data base required finding a more functional and user-friendly data base management system. This was done by creating the Data Management Office (DMO), after much discussion and surveys of CRDEC's data base requirements, and by purchasing the Molecular Access System (MACCS) (Version 5.14, marketed by Molecular Design, Ltd.) data base management system and the VAX Rdb/VMS Version 2.1 (Digital Equipment Corporation, Maynard, MA) for installation on a dedicated VAX 780. MACCS is a user-friendly, menu-driven, chemical- oriented system that should fulfill CRDEC's chemical data basing needs. It meets all the requirements for the CASDC and offers additional capability in structure storage and structure/substructure retrieval. Each compound entered into the data base must have its structure defined, or no structure available specified, before it can be registered. Structure storage is required to remove any doubt about a compound's identity. This allows anyone wishing to query for complete structures or substructure fragments to be able to exactly match the structural features they define.

3. ACCESSIBILITY

3.1 Eligibility and Passwords

The CASDC is available to CRDEC, DOD services, other government agencies, and their contractors having a requirement for simulant related data. Individuals not having a need for frequent access can obtain information, have their queries processed, and have printed data mailed by contacting Phillip Coon, the CASDC data base manager, or his alternate George Famini at the following address:

Commander
U.S. Army Chemical Research, Development
and Engineering Center
ATTN: SMCCR-RSP-C
Aberdeen Proving Ground, MD 21010-5423

Commercial telephone inquiries can dial (301)671-3248/2775, whereas AUTOVON network can use 584-3248/2775. Those requiring frequent use and desiring a password must contact the DMO at the following address:

Commander
U.S. Army Chemical Research, Development
and Engineering Center
ATTN: SMCCR-TDT/Steve Lawhorne
Aberdeen Proving Ground, MD 21010-5423 Commercial telephone inquires to the DMO can dial (301)671-2938 or AUTOVON users dial 584-2938.

3.2 Data Base Access

The DMO computer can be accessed by selecting 2-DMO from the CRDEC workplace automation PACXNET of available systems. The remote long distance number into the CRDEC PACXNET is 1-800-826-3460. The DMO computer can be accessed directly from locations having TELNET service. Typing (open crdec-dmo.apgea.army.mila) at the TELNET prompt provides this direct access. As previously mentioned, a valid user id and password from the DMO is required. Typing "menu" at the dmo prompt provides the DMO menu of data bases (Figure 1). Selecting option 2, "Simulants," accesses the CASDC menu of options (Figure 2). Use this menu to conduct searches, generate data reports for compounds of choice, or to exit to the DMO menu.

3.3 Conducting Searches

Different approaches can be used in executing queries within the MACCS system. A query can use different options in search of specific data. The reasons for selecting certain query paths depend on your wish to identify certain compounds or to retrieve data points. The following search strategy is an abridgement of the available options and represents a simple approach to data retrieval. MACCS offers 38 pages under "(H)ELP" to assist in executing all system options.

After selecting option 1, in order to conduct a data search, the user is presented with the EXECUTIVE MODE menu of MACCS (Figure 3). Input can be either "(g)raphics" (default) using a cursor control device or "(k)eyboard" when in EXECUTIVE MODE. The option modes for conducting data searches are "(S)EARCH," "(D)ATA," and "(F)IND." Query results in SEARCH MODE (Figure 4) display internal and external registry numbers and compound name. A listing is also created that can be used as the reference list for further data searches. The lists are also used in data manipulation and transfer. Query results in DATA MODE (Figure 5) display entry numbers, datatype name and number, and any accompanying data without identifying the compound by name. No further treatment of the output can be conducted as no lists are created. Although data searches can be conducted in DATA MODE, its primary function is data entry, deletion, manipulation, and transfer. DATA MODE is also used to view individual data points for compounds identified in SEARCH MODE. To display a listing of datatypes, acquire datatype entry numbers, determine units of measure or to preview comments, select "(D)ATA" and then "(I)ndex." After the "datatypes=" prompt, specify the datatype number(s), a range of numbers, or (all) for a complete listing.

CRDEC Data Base Management System

1. Fate & Effects Data Base
2. Simulants Data Base (MACCS)
3. ILO Chemical & Physical Properties (MACCS)
4. ILO Toxicity Screening Data Base
5. EPA Safety Data Sheets
6. Chemical/Physical Properties Data Base
7. Chemical Hazard Response Information System (CHRIS)
8. Set a new password
9. Send comments or questions to the system manager
10. Exit

Enter the number corresponding to your choice: 2

Figure 1. DMO MENU

Chemical Agent Simulant Data Center
and Report Generator

Questions or Comments should be Directed to
Phillip Coon (3248/3518) or George Famini (2670/3518)

1. Enter Chemical Agent Simulant Data Center (MACCS)
2. Enter Report Generator of Chemical Agent Simulant Data Center
3. Locate Citations for References to Data Values
4. Exit the Simulant Data Center

Please enter your choice>

Figure 2. CASDC MENU

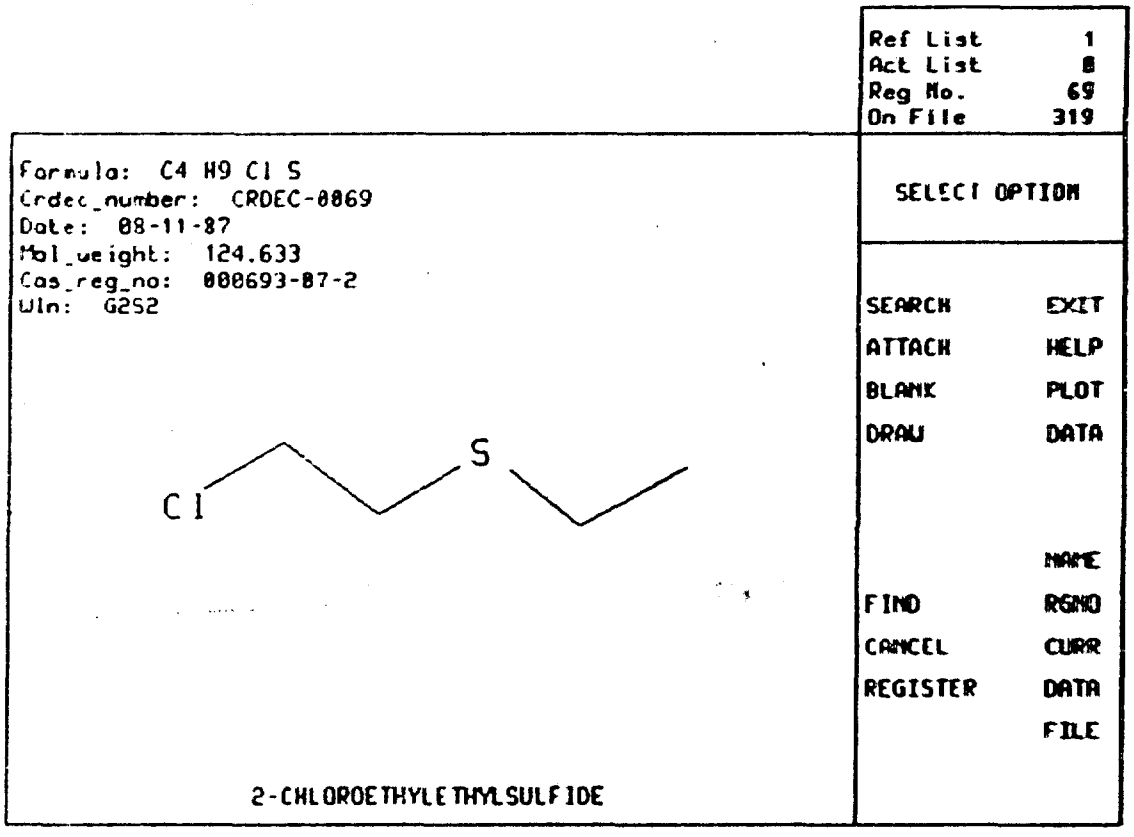


Figure 3. EXECUTIVE MENU

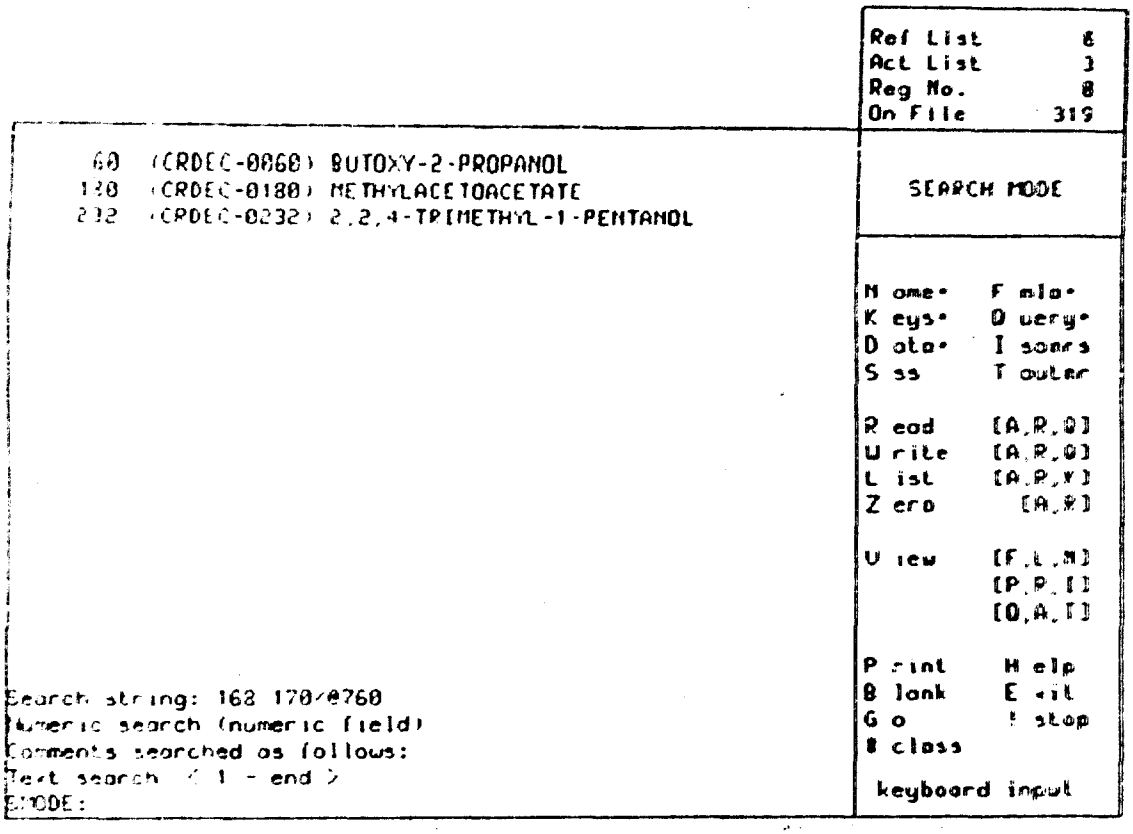


Figure 4. SEARCH MODE MENU

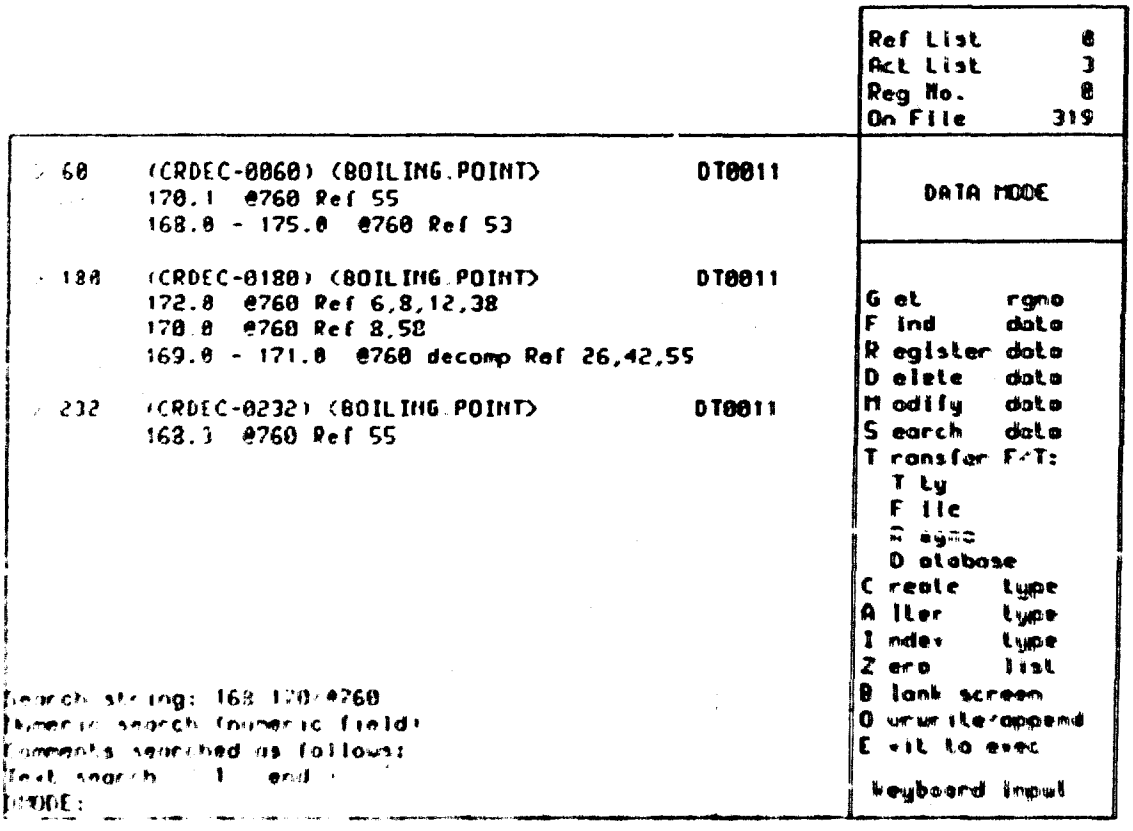


Figure 5. DATA MODE MENU

3.3.1 Name Searches

Chemical names can be searched in two ways. The first uses the "(F)IND (N)AME" option in EXECUTIVE MODE or "(N)ame" option in SEARCH MODE. This queries the IUPAC convention name that is entered at the time a structure is registered. Name fragment searches use the @ sign before and/or after a name fragment as a universal substitute. A second method can be used if no compounds are selected using NAME options. This method searches "(d)atatype 7," *Synonyms*, in "(S)EARCH" or "(D)ATA" MODE. Synonyms include all other names and identifiers. No @ sign is required for synonyms. Synonyms are a textual search descriptor that recognizes any character string. Typing "(e)xit" when in SEARCH or DATA MODE will return the user to EXECUTIVE MODE.

3.3.2 Data Searches

Data searches for numeric or text data are best conducted in "(S)EARCH" MODE, using the "(D)ata" option. The user will be able to identify compounds by name and to generate lists. Specific data values can then be examined in "(D)ATA" MODE or by using "(F)IND (D)ATA." A data search in "(D)ATA" MODE using the "(S)earch" option will not identify a compound by name. Figure 5 shows data retrieved using this option. Data searches are always done on the Reference List unless it is zero; in which case the search is done on all compounds in the data base. To zero lists, select "(Z)ero (R)eference" or "(A)ctive" when in SEARCH MODE or "(Z)ero" when in DATA MODE. Numeric searches are made by identifying the datatype number at the prompt then specifying a from/to range separated with a space or dash. Dependent variables or any other item in the comment field can be specified by using a slash and the desired character string immediately after the upper bound. An example of a query range for normal boiling point would be "168 170/@760." Figures 4 and 5 show the contrasting results of this query in SEARCH MODE and DATA MODE respectively. Sometimes it is advisable not to specify dependent variables, as some data have dependent variables unstated. Dependent variables and comments can be scrutinized after a listing is generated.

Searching of multiple datatypes with a single query cannot be executed. Searching for more than one property must be done sequentially in SEARCH MODE. After the initial property search, the resulting listing, or active list, becomes the reference list by selecting "(R)ead (R)eference" and then typing "act." This is done each time the active list is to become the reference list. The reference list remains until it is zeroed. Table 2 is an example of a multiple property search for a mustard simulant showing properties, ranges, available compounds, and number of

TABLE 2. SEQUENTIAL SEARCH

EXAMPLE OF SEQUENTIAL PROPERTY SEARCH FOR HD SIMULANT

PRIORITY LIST	PROPERTY	DATA TYPE NUMBER	RANGE	AVAILABLE COMPOUNDS	HITS
1	MOLECULAR WEIGHT	3	143 - 175	319	88
2	BOILING POINT	11	196 - 239	88	29
3	VAPOR PRESSURE	8	0.05 - 0.50	29	15
4	SOLUBILITY PARAMETER	34	9.54 - 11.66	15	4
5	DENSITY	9	1.14 - 1.40	4	2
6	SURFACE TENSION	14	38.7 - 47.3	2	1

TABLE 3. HD AND MS DATA

PROPERTY COMPARISONS FOR HD AND METHYL SALICYLATE

PRIORITY LIST	PROPERTY	HD	METHYL SALICYLATE
1	MOLECULAR WEIGHT	159.1	152.2
2	BOILING POINT	217	223
3	VAPOR PRESSURE	0.069	0.13
4	SOLUBILITY PARAMETER	10.6	10.6
5	DENSITY	1.2739	1.1738
6	SURFACE TENSION	43.2	38.8

qualifying compounds. All properties have a range of ±10% except vapor pressure. The table demonstrates how the initial 319 compounds are diminished each time a new property is queried. The final selection was methyl salicylate. Table 3 is a comparison of the six selected property values for mustard and methyl salicylate.

3.4 Generating Reports

The CASDC provides a means of generating reports of all compiled data for compounds of interest resulting from a data search. The report format was created using DATACCS, which is external to MACCS and located on the DMO VAX 780. A five-page report was required to accommodate all the datatypes. After completing a data search the user exits MACCS by typing or selecting the "(E)XIT" option while in EXECUTIVE MODE and is returned to the CASDC menu (Figure 2). With a list of entry numbers for compounds of interest in hand, the user selects option 2 and states the type of terminal in use as requested. At this point, the user is requested to enter the entry number for the compound of interest. A <RET> is used to generate each page of the report. Type "(e)xit" after the last page to return to CASDC menu This procedure is repeated for each compound for which a report is desired. Figures 6-10 are examples of a complete report of the mustard simulant methyl salicylate. The user ends the session by selecting the "quit" option of the CASDC menu, the "quit" option of the DMO menu, and logs off with a "lo" at the dmo prompt.

4. SUMMARY AND DISCUSSION

Personnel at CRDEC (CBM Branch) established the CASDC. These personnei are responsible for data base maintenance and frequently add new compounds, new data points, or define new datatypes. The CASDC is an on-line, user-friendly, computerized data base of compounds that have been used, recommended, screened, or otherwise considered as chemical agent simulants. The data base is available to CRDEC, other DOD services, other government agencies, and contractors engaged in simulant research. Currently, there are 600 compounds entered with 50 different types of data that can be requested. Available to the user is a report generator that provides a copy of all compiled data for compounds of interest. New compounds, data, and datatypes are added as they are encountered or as requests are received for inclusion.

Along with identifying and entering new data, the data base compilers are developing new descriptors to better define simulant applications and selection criteria. The data base managers expect that requests for simulant use, application, selection criteria, agent/simulant correlation or other similar data will generate a report similar to Figure 11.

CHEMICAL AGENT SIMULANT DATA CENTER

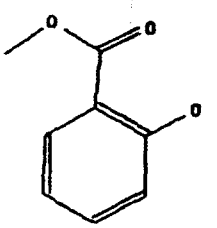
Entry Number 194	Structure 
CRDEC Number CRDEC-0194	
CAS Reg Number 000119-36-8	
Formula C8 H8 O3	
Molecular Weight 152.151	METHYL SALICYLATE
WLN QR BVO1	Synonyms
Today's Date 01/22/88	wintergreen oil 2-hydroxybenzoic acid methyl ester
Page 1 of 5	

Figure 6. SIMULANT REPORT PAGE 1

CHEMICAL AGENT SIMULANT DATA CENTER

METHYL SALICYLATE	Vapor Density 5.24 Ref 55,64	Molar Volume 128.94
Vapor Pressure [torr] 0.13 @20C Ref 55 0.165 @25C Ref 53 0.891 @28C Ref 79 1.0 @54C Ref Chem Eng Hnbk 40.0 @126.2C Ref Chem Eng HnbK 400.0 @197.5C Ref Chem Eng Hnbk	Melting Point [C] -8.6 Ref 42,64	Calc Molar Ref 39.58 Ref 85
	Viscosity [cp]	
Density [gm/cc] 1.1738 @20C Ref 55,64 1.182 @25C Ref 79	9.7 @20C Ref 64 est	
	Volatility [mg/m3]	
Boiling Point [C] 228.0 - 224.6 @760 Ref 42,55,64 222.9 @760 Ref 79	1060.0 @25C Ref 54 556.0 @28C Ref 79	
	Diffusivity [cm2/sec]	
Surface Tension [dynes/cm] 39.9 @25C Ref 72		
	Refractive Index	
Page 2 of 5	Entry Number 194	1.5385 @20C Ref 42

Figure 7. SIMULANT REPORT PAGE 2

CHEMICAL AGENT SIMULANT DATA CENTER

METHYL SALICYLATE

Heat of Vaporization [cal/gm]

59.4 @25C Ref 79
83.2 Ref 53

Heat of Combustion [cal/gm]

8986.0 Ref 53

Heat of Fusion [cal/gm]

Heat of Formation [cal/gm]

Energy to Vaporize [cal/gm]

Heat Capacity [cal/gm degC]

Specific Heat [cal/gm]

Decomp Temp [C]

Oxygen Index

Flash Point [C]
181.1 closed cup Ref 55,64,79
99.0 closed cup Ref 42

Autoignition Temp [C]

Dielectric Constant

9.41 @30C Ref Dean

Dipole Moment [debyes]

2.23 @20C Ref 80
2.53 @25C Ref Dean

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Entry Number 194

Figure 8. SIMULANT REPORT PAGE 3

CHEMICAL AGENT SIMULANT DATA CENTER

METHYL SALICYLATE

Hygroscopicity

Critical Temp [C]

Critical Pressure [atm]

Critical Volume [cc/mole]

Critical Density [gm/cc]

O/W Partition Coefficient [LogP]
2.46 Ref 72
2.55 Ref 72 (selected)

Solubility Parameter [N]

18.6 Ref 79

Toxicity
LD50,oral,rat-0.887gm/kg Ref 55
LD50,oral,rabbit-2.8gm/kg Ref 55
LD50,oral,dog-2.1gm/kg Ref 55
inh,rat,28 7hr exps at 700mg/m3-no effect Ref 64
avg LD human child-10ml Ref 42,64
avg LD human adult-30ml Ref 42,64
acceptable daily intake-500micrograms/kg Ref 64

Water Solubility

slight

Solubility Value [gm/ml]

0.87 @30C Ref 42,79

Hydrolysis Rate

Industrial Application
used as flavorant
used in perfumes
used as analgesic

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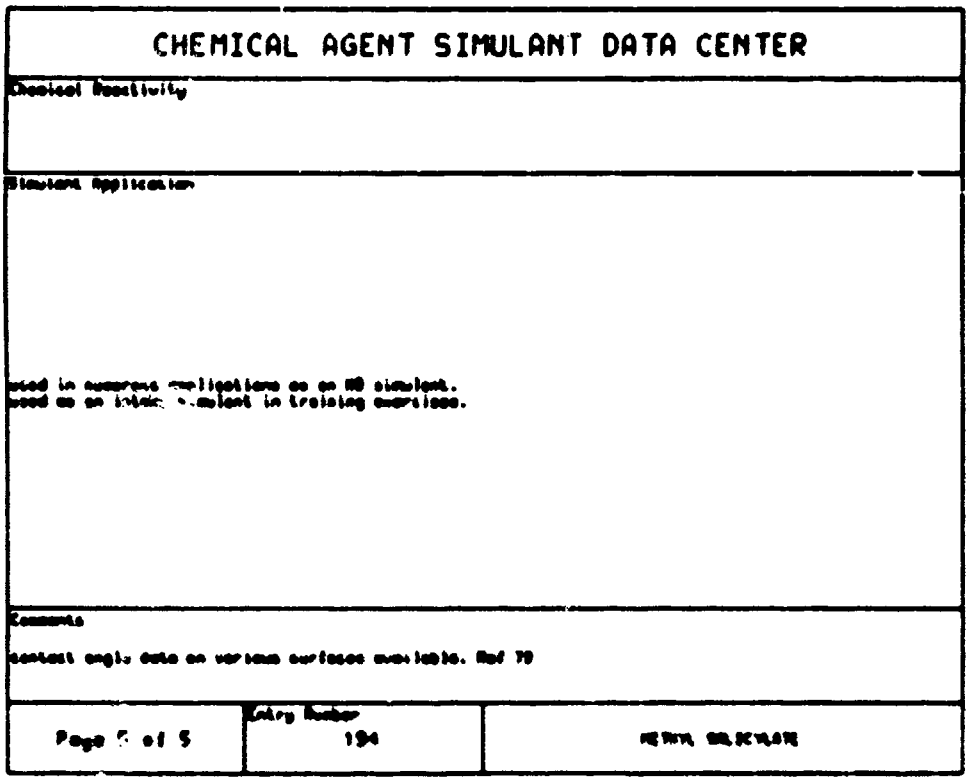
Entry Number 194

Figure 9. SIMULANT REPORT PAGE 4


CHEMICAL AGENT SIMULANT DATA CENTER

Chemical Reactivity

Simulant Application

used in numerous applications as an HD simulant.
used as an initial simulant in training exercises.

Comments

contact angle data on various surfaces available. Ref 79

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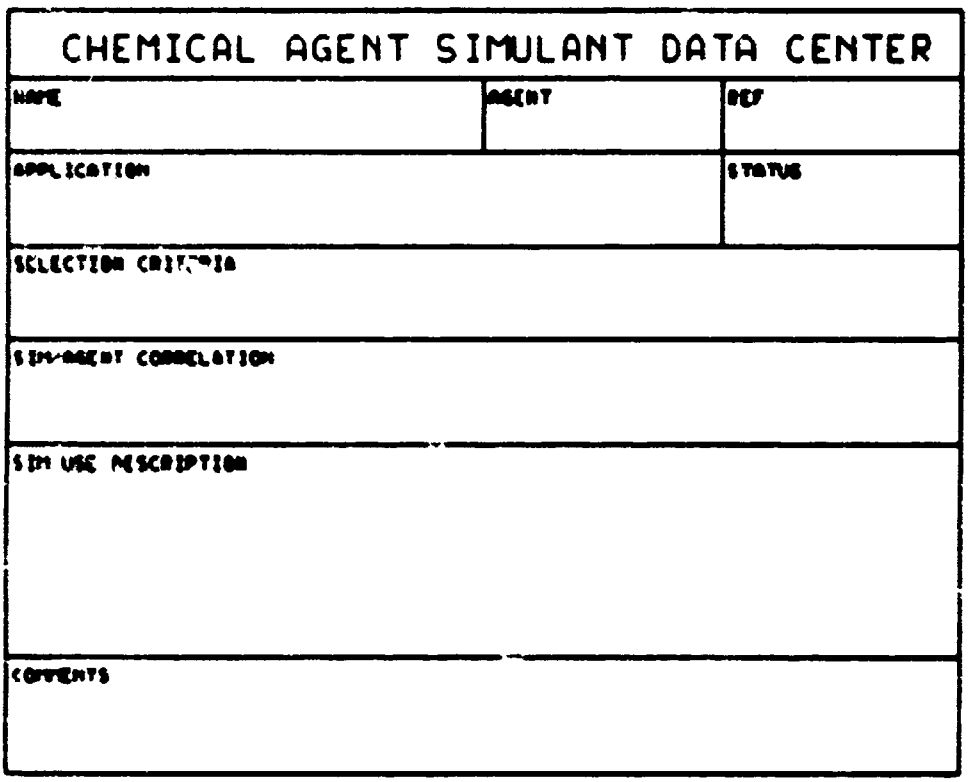
Figure 10. SIMULANT REPORT PAGE 5


CHEMICAL AGENT SIMULANT DATA CENTER

NAME | AGENT | REF

APPLICATION | STATUS

SELECTION CRITERIA

SIM-AGENT CORRELATION

SIM USE DESCRIPTION

COMMENTS

Figure 11. SIMULANT USE REPORT

Personnel responsible for the CASDC solicit all individuals having comments for improving the data base to offer their recommendations. This is the principle way that the CASDC can be updated. Your imput will ensure that the data base reflects state-of-the-art in simulant research and that all pertinent compounds are entered into the data base.

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APPENDIX
DATA DICTIONARY

- Name: an unassigned fixed datatype established at the time a compound is registered. To assure continuity, an effort is made to follow rules of nomenclature as established by The Council of the International Union of Pure and Applied Chemistry (IUPAC).[1] A name search is done under NAME option of SEARCH mode or FIND NAME option of EXECUTIVE mode. If not found, a search should be made of synonyms under SEARCH or DATA mode.

- Formula: empirical formula of compounds following the Hill convention. It is an unassigned fixed datatype. It is system generated at time of registration and is accessed under FORMULA option of SEARCH mode.

1. CRDEC Number (External Registry Number): externally assigned fixed datatype that will identify the compound throughout all CRDEC data bases. Some coordination is required between Data Management Office and data base generators to ensure the singularity of this identifier. All data bases on the system should be queried for this compound to determine if a CRDEC number has been assigned or needs to be assigned.

2. Date Entered: a system generated fixed datatype that represents the date the compound was initially registered. It uses American format of MM/DD/YY.

3. Molecular Weight: a fixed datatype that is the sum of atomic weights of all atoms in the molecule based on Carbon 12. It is system generated, and units are understood as grams per mole (g/mol).

4. CAS Registry Number: a singular identifier assigned by Chemical Abstract Service and represents the most universal code for compound identification used throughout the chemical industry.[2] CAS was established in 1965, and over 4 million substances have been registered. It is a formatted field using the form 00000-00-0 with leading zeros omitted.

5. Wiswesser Line-Notation (WLN): this is an important indexing tool that establishes the topology and make-up of a molecule using an unambiguous code.[2] Many compilations are indexed using WLN, and some computerized data bases access or generate structures using this line code. It is a text field and can be used for accessing certain compounds or querying for various structural features.

6. Military Designation: this descriptor was designed to reserve a fixed datatype for future use and contains no data.

7. Synonyms: a listing of other chemical names, trade names, code names, abbreviations, acronyms, etc. If a compound is not found under the NAME option of SEARCH or FIND mode, it can be searched under this datatype using a full name or name character string.

8. Vapor Pressure: the pressure exerted by a substance in equilibrium with its own vapor.[3] It is temperature dependent and increases with an increase in temperature and whose standard unit is millimeters of mercury (mmHg), also called Torr. CRDEC has compiled estimation routines using various procedures. These data are used until experimental data are encountered.

9. Density: the mass of a substance that is temperature dependent and whose units are grams per cubic centimeter. It is understood to be equivalent to specific gravity (ratio of equal mass to water at 4 °C) when a singie temperature is cited, otherwise the comparing temperature of water is the second temperature cited following the slash.

10. Vapor Density: the ratio of equal volumes of vapor and dry air under identical conditions of temperature and pressure. It can be calculated as the molecular weight of the chemical divided by that of dry air that has been approximated to be 29.[4] The result is the ratio of chemical vapor to that of air and, therefore, is unitless.

11. Boiling Point: the temperature at which the vapor pressure of a chemical is in equilibrium with the surrounding system and is pressure dependent. All

boiling points have their requisite pressures stated. Normal boiling points within a range can be searched by typing /760 immediately after the upper bound. Units are in degrees Celsius.

12. Melting Point: the temperature at which a substance changes from a solid to a liquid. It is generally equivalent to the freezing point or is specified as a range. This datatype can be used to ascertain if a chemical is liquid or solid. Units are in degrees Celsius.

13. Molar Volume: volume occupied by 1 mole and is equal to the molecular weight divided by the density.[1] Units are cubic centimeters per mole.

14. Surface Tension: the force exerted on the plane of the surface per unit length that opposes spreading and tends to shape liquids into drops.[5] Values are expressed in dynes per centimeter and decrease with an increase in temperature. In the absence of literature values, the estimation method of MacLeod and Sugden is used.

15. Liquid Viscosity: the measure of liquid resistance to a change of form or a form of internal friction.[1] It is expressed in dyne-seconds per square centimeters or poise. Kinematic viscosity is the ratio of viscosity to density and whose unit is the stoke. Stokes are converted to poise by multiplying by density at the given temperature. Viscosity estimation is done using Chemest; a computer package based on the Handbook of Chemical Property Estimation Methods using the method of Orrick and Erbar.

16. Vapor Viscosity: same as liquid viscosity with unit expressed in micropoise.

17. Volatility: the mass of saturated vapor concentration measured in milligrams per cubic meter. It is also known as the saturated vapor density or concentration. It can be calculated from vapor pressure (VP) and molecular weight (MW) data with temperature (T) in Kelvin degrees using the equation:[4]

$$Volatility = \frac{VP \times MW \times 16020}{T} \qquad (1)$$

18. Diffusion Coefficient: a transport property that measures the flux across a plain of binary gas concentration gradients.[6] It is the diffusion of chemical vapor in air measured in square centimeters per second.

19. Refractive Index: the ratio of the velocity of light in a vacuum to its velocity in the substance.[5] The light source is the sodium D line and is a dimensionless parameter ranging from 1.3 to 1.5 for organic liquids. Also called index of refraction, absolute index of refraction, absolute refractive index, or refractivity. It is a function of wavelength, temperature, and pressure.

20. Molar Refraction: a parameter indicating the way that a molecule interacts with light. It is calculated from the equation:[7]

$$M_R = \left(\frac{n^2-1}{n^2+2}\right)\frac{MW}{d} \qquad (2)$$

n = refractive index
MW = molecular weight
d = density

21. Decomposition Temperature: the temperature at which a chemical decomposes or separates into two or more different substances. Units are degrees Celsius.

22. Flash Point: the temperature that a volatile combustible substance will ignite when exposed to a flame. Two methods commonly used are the Tag closed cup (cc) or the Cleveland open cup (oc) which is usually slightly higher than the closed cup method.[8] Units are degrees Celsius.

23. Autoignition Temperature: the temperature at which a substance will ignite without an ignition source such as flame or spark and measured in degrees Celsius.

24. Oxygen Index: the percentage of oxygen in nitrogen that will cause a chemical to sustain a candle type flame when the gas is passed up and around the chemical.[9] It is used as a flammability or flash indicator.

25. Heat of Vaporization: the quantity of heat necessary to change one gram of liquid to vapor without a change of temperature[8], measured in calories per gram. It varies with temperature and is normally stated at the boiling point with slightly higher values at ambient temperatures. Also called the latent heat of vaporization, heat of evaporation, or enthalpy of vaporization. CRDEC employs various estimation methods for this property depending on the availability of other data.

26. Heat of Combustion: the amount of heat generated by the combustion of one gram mole weight of the substance measured in calories per gram.[1]

27. Heat of Fusion: the quantity of heat necessary to change one gram of solid to a liquid with no temperature change measured in calories per gram.[5] Also termed latent heat of fusion, enthalpy of fusion, or enthalpy of melting.

28. Heat of Formation: the quantity of heat involved in the formation of 1 mol of substance from its elements in their standard states, measured in calories per gram.[3] A negative sign preceding the value signifies heat is evolved and no sign or positive sign shows that heat is absorbed.

29. Energy of Vaporization: equivalent to heat of vaporization minus any work done, measured in calories per gram. Can be calculated as the heat of vaporization in calories per gram mole minus the gas constant (1.987 cal/mol-degree) times the temperature in Kelvin.

30. Heat Capacity: the quantity of heat required to increase the temperature of a substance one degree.[7] It is the ratio of absorbed heat to the resulting temperature increase. Units of measure are calories per degree Celsius.

31. Specific Heat: the term historically meant the ratio of heat capacity of a substance to that of an equal mass of water. Recently, it meant the ratio of heat capacity to the mass of a substance and could more appropriately be called the specific thermal capacity [3]. When measured in calories per gram degree Celsius it is equivalent to the historic older definition. Specific heats should be specified as being measured under constant conditions of volume and pressure.

32. Hydrolysis Rate: the decomposition of a compound by reaction with water. A text datatype to accommodate various methods of measurement that are temperature, time, and pH dependent. Because of various reporting conventions, a search of other related solubility properties should be done when trying to match agent/simulant hydrolysis rates. After a compound has been identified, determine if hydrolysis data is available. It is planned to include other parameters describing solvent/solute interactions.

33. Octanol/Water Partition Coefficient: the ratio of chemical concentration in the octanol phase to its concentration in the aqueous phase of a two-phase octanol/water system. Values are unitless, may be positive or negative, and range from -3 to 7.[8] Partition coefficient are useful in modeling chemical transport through biological systems and in studies of environmental fate. CRDEC has computerized estimation routines for this property.

34. Hildebrandt Solubility Parameter: a quantitative measure of solubility for nonpolar organic compounds calculated as the square root of the cohesive energy density, and defined as solubility parameter (H). It can be calculated using data with the following equation:

$$\delta_H = \left[\frac{d(\Delta H_v - RT)}{MW}\right]^{1/2} \qquad (3)$$

d	=	density (g/cm)
ΔH_v	=	heat of vaporization (cal/g mole)
R	=	gas constant (1.987)
T	=	temperature (K of density)
MW	=	molecular weight

Some consideration must be given more polar or hydrogen-bonded solvents because of the presents of stronger intermolecular forces.

35. Hygroscopicity: the ability to become wet by absorption of water from the atmosphere. Data is generally qualitative expressed as yes or no with quantitative data compiled when available.

36. Water Solubility: this text datatype is for qualitative data of unsoluble, slight, soluble, and miscible categories.

37. Water Solubility Value: a quantitative measure of water solubility expressed in grams per 100 mL. The highly dependent temperature variable is included when available.

38. Critical Temperature: the temperature above when a substance cannot exist in the liquid phase, regardless of the pressure.[5] Units are degrees Celsius.

39. Critical Pressure: the pressure required to liquefy a gas at the critical temperature[5]. Units are atmospheres (atm).

40. Critical Volume: the volume occupied by one gram of liquid or gas at its critical temperature and critical pressure[5]. Units of measure are in cubic centimeters per mole.

41. Critical Density: the density of a substance at its critical temperature and critical pressure[5] as measured in grams per cubic centimeter.

42. Dielectric Constant: the ratio of the capacity of a condenser with that substance as dielectric to the capacity of the same condenser with a vacuum for dielectric.[1] It is a measure of the amount of electrical charge a substance can withstand at a given electric field strength. This property is temperature and frequency dependent and units are dimensionless.

43. Dipole Moment: the summary or permanent dipole moment is dependent on the magnitude of the charge and distance separating positive and negative charges. It is the summary of both electrons and nuclei charges in the molecule. Numerical values are expressed in debyes, which are equivalent to 10-18 electrostatic units per centimeter $(esu\text{-}cm)^5$. Dipole moments of organic molecules normally fall between 0 and 5 debyes.

44. Toxicity: a listing of various values to indicate relative toxicity. This topic is a data base unto itself, and the requirement for detailed toxicity data can be better served through access to existing toxicity data bases.

45. Chemical Reactivity: a text descriptor originally designed for materials compatibility data. It was recently expanded to include all types of reactivity data with other chemical compounds, groups, and classes. Little data has been entered on this subject because it requires searching through other than simulant related-literature.

46. Simulant Application: text data designed to describe the relevance of the compound to simulant research. Information on this topic is currently limited to simulated agent and application with many compounds having no data. It is planned to expand this with additional datatypes for agent simulated; type of research activity; selection criteria; simulant/agent correlation; research methods; efficacy; and status to describe if the simulant was used, recommended, screened, or not recommended. Each compound in the data base should have at least one entry for this descriptor.

47. Industrial Application: a description of the application and prevalence of the chemical in the private sector. This will assist simulant users in determining data sources and likelihood of acquiring use approvals.

48. Comments: the location for data not specifically related to the datatypes previously described.

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